Scanning tunnelling microscopy for ultracold atoms

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We propose a novel experimental probe for cold atomic gases analogous to the scanning tunnelling microscope (STM) in condensed matter. This probe uses the coherent coupling of a single particle to the system. Depending on the measurement sequence, our probe allows to either obtain the *local* density, with a resolution on the nanometer scale, or the single particle correlation function in real time. We discuss applications of this scheme to the various possible phases for a two dimensional Hubbard system of fermions in an optical lattice.

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Recent advances in the field of ultracold atoms have led to a close connection between quantum gases and condensed matter physics. The achievement of strongly correlated systems and their remarkable tunability open the possibility to realize 'quantum simulators' for quantum many-body phenomena. To name one example, ultracold fermionic systems clarified the crossover between a BCS-state of paired fermions to a Bose-Einstein condensate of ultracold bosonic molecules [1, 2, 3, 4, 5]. Further investigations of strongly correlated systems were initialized by the successful loading of ultracold bosonic [6] and fermionic [7] atoms into three-dimensional optical lattices. In these periodic lattice potentials created by counter-propagating laser beams the physics of different lattice models can be mimicked [8, 9]. In particular the fermionic Hubbard model, which plays an important role on the way of understanding high-temperature superconductivity, can be realized naturally given the short range nature of the interactions between the neutral atoms.

Whereas achieving the exotic quantum phases experimentally appears feasible with today's technology their clear identification remains an obstacle. Compared to condensed matter the neutrality of the cold atoms is both an advantage and a drawback since they cannot be perturbed as easily as electrons in a solid. Possible probes are thus more sophisticated than their condensed matter counterparts. In addition, for ultracold atomic gases an inhomogeneous confining potential causes the coexistence of different spatially separated quantum phases [8, 10, 11]. This makes their realization and observation in the presence of a trapping potential very involved and creates a need for a method of probing the systems locally. However, the existing probes [10, 11] still involve an averaging over regions of various densities and new techniques which allow for a local detection need to be developed.

In condensed matter physics, a remarkable local probe was provided by the scanning tunneling microscope (STM) [12]. It allowed to explore and image the surface topography with atomic resolution, paving the way to control and analyze quantum phenomena on solid surfaces [13]. In addition to the density analysis with unprecedented resolution, the STM has also become a spectroscopic tool probing the local density of states. This spectroscopic method had a major impact on the understanding of the physical properties of strongly correlated systems for which the local density of states provides unique information on the physics of the system. In particular the STM has made significant contributions to the field of high temperature superconductors [14].

In this work we propose a novel experimental setup to locally probe cold atomic systems in an approach similar to and as versatile as the STM. The probe relies on the coupling of a single particle to the system. Different 'operating modes' yield either a measurement of the local density or of the single particle Green's function in time. The realization of such a probe will open the possibilities to investigate exotic quantum phases in great detail as we show on the example of the Hubbard model. In extension to the conventional STM in condensed matter physics our scheme would allow for measurements in a three-dimensional sample.

The key idea for the realization of an STM-like scheme with cold atoms, the 'cold atom tunneling microscope' is sketched in Fig. 1. A single trapped particle is used as a probe of local quantities by inducing a controlled interaction between the probe particle and the quantum many-body state. To allow for a precise control over the motion of the probe and to facilitate a convenient readout mechanism, we suggest to employ a single atomic ion trapped in the vibrational ground state of a radio-frequency Paul trap [15]. In this case the spatial resolution of the microscope relies on the excellent control over the position and motion of trapped ions on the sub-micron scale. However, the working principle of the microscope does not depend on the charge of the probe particle and it also applies to a neutral atomic quantum dot [16] provided that the trapping potential of the dot has only a negligible influence

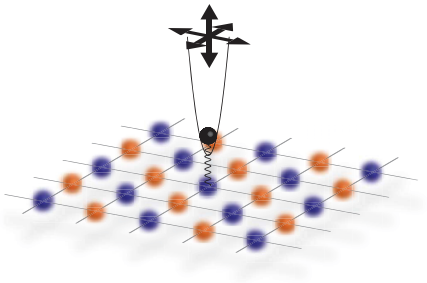

FIG. 1: Sketch of the cold atom tunneling microscope. As an example the application to an anti-ferromagnetic state with alternating spin states labeled by different colors is shown.

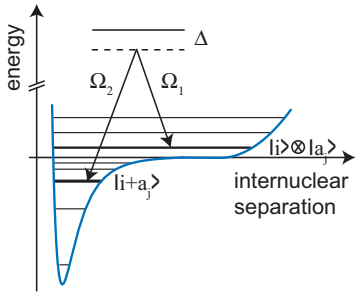

FIG. 2: Two-photon Raman coupling of the ion $|i\rangle$ and an atom $|a_j\rangle$ in a harmonic potential well to a molecular ion bound state $|i + a_j\rangle$. The single photon coupling is detuned by Δ from a resonant transition to suppress spontaneous emission from the intermediate excited state. The effective two-photon Rabi frequency Ω_0 is proportional to the coefficients of the single photon transitions and inversely proportional to the detuning Δ, i.e. $\Omega_0 \propto \Omega_1\Omega_2/\Delta$.

on the quantum many-body system [17]. The controlled interaction between the probe particle (the ion) and the quantum many-body system could be provided by a two-photon Raman coupling.

As we show below the cold atom tunnelling microscope facilitates a local detection of the density on individual lattice sites and, quite remarkably, it even allows to perform a spin-resolved detection of the density. The realization of a spin-resolved STM is a long-sought goal in condensed matter systems but has not yet been achieved. The cold atom tunnelling microscope also allows to perform spectroscopy by observing the local single particle Green's function $\langle c^\dagger_{\sigma,j}(t_0)c_{\sigma,j}(0)\rangle_F$ in time. Here $c_{\sigma,j}$ is the annihilation operator for the neutral atom on a site j with spin $\sigma = \{\uparrow, \downarrow\}$ and $\langle\cdot\rangle_F$ stands for taking the expectation value with respect to the atomic system only. The temporal decay of this function directly reflects the nature of the excitations and gives thus direct information on the quantum phases present in the system.

We first show taking the example of fermionic atoms in two different spin states $\uparrow$ and $\downarrow$ in an optical lattice how a measurement of the local density, the 'scanning mode', can be achieved. It is facilitated by a two-photon Raman coupling between the ion $|i\rangle$ and an atom $|a_j\rangle$ in a lattice well j by which a weakly bound molecular ion $|i+a_j\rangle$ can be created (see Fig. 2). This coupling can be described by the expression $\left(\sum_\sigma \Omega_\sigma(t)M^\dagger_\sigma I c_{\sigma,j} + h.c.\right)$. Here M_σ and I are the annihilation operators for the molecular ion and the atomic ion, respectively. The coupling strength $\Omega_\sigma(t)$ can be controlled experimentally. By choosing the correct frequency and polarization of the laser fields, the coupling is dependent on the atomic 'spin' state paving the way for the spin-resolved microscopy.

The experimental sequence to detect the local density is as follows: At time $t = 0$ the atomic many-body system is prepared in its ground state $|\Psi_0\rangle$. The ion is introduced into the lattice well j in state $|i\rangle$ and the Raman coupling is switched on for a duration δt, i.e. $\Omega_\sigma(t) = \Omega_{\sigma,0}$ if $t \in [0, \delta t]$ and vanishes otherwise. The time δt has to be short compared to the internal time-scales of the probed system (i.e. time-scales set by the atom-atom interaction U, the kinetic energy of the atoms J, and the atom-ion contact interaction U_{ai}) to avoid a change of the many-body state during the probe sequence. The Raman coupling generates a superposition of the initial state $|\Psi_0\rangle \otimes |i\rangle$ and the state $c_{\sigma,j}|\Psi_0\rangle \otimes |i + a_j\rangle$ in which one atom is removed from the system and a molecular ion is formed. The ratio between the amplitudes of the two states depends on the density of atoms in the well j. Hence detecting the probability (i.e. the average of the outcome of several quantum measurements) for molecule formation after the application of the Raman pulse measures the local density of atoms in the lattice well j by the relation $\langle\sum_\sigma M^\dagger_\sigma M_\sigma\rangle = \sum_\sigma \sin^2(\Omega_{\sigma,0}\delta t)\langle n_{\sigma,j}\rangle_F$ with $\langle n_{\sigma,j}\rangle$ the local atomic density. The outcome of the photo-association process can be detected by measuring the changed oscillation frequency of the heavier molecular ion in the Paul trap or by observing the absence of resonant light scattering of the molecular ion and its reappearance after photo-dissociation [18]. The procedure can be repeated scanning different lattice sites as sketched in Fig. 1 with a spatial resolution on the order of 20 nm [19]. To facilitate the measurement of the density with a good signal to noise ratio, the lattice potential could be increased such that the density profile on different lattice sites is frozen and sequential measurements on single lattice site are feasible.

Using the cold atom tunnelling microscope with a different sequence, the 'tunneling mode', allows to perform spectroscopy and to measure time dependent correlations locally. The experimental sequence is sketched in Fig. 3. As in the scanning mode we start at $t = 0$ in the state $|\Psi_0\rangle \otimes |i\rangle$, i.e. the ground state $|\Psi_0\rangle$ of the atomic system and a single atomic ion. A two-photon Raman process is applied over a short time interval δt_1 to couple the ion with an atom present in the lattice well. Sub-

sequently, the superposition state of the atomic and the molecular ion $|i\rangle + \alpha|i + a_j\rangle$ is removed from the system such that they are non-interacting with the remaining quantum many-body system, for example their center-of-mass position can be shifted by applying a small dc voltage. After a variable time of free evolution t_0 in this isolated position they return into the addressed lattice well and the application of the two-photon Raman process is repeated for a time interval δt_2. The outcome of the molecule formation is detected afterwards [28]:

$$\begin{aligned}\langle M^\dagger M\rangle &= A(\delta t_1,\delta t_2) + \sin^2(\delta t_2\Omega_0)\left[\cos(\delta t_1\Omega_0)-1\right]\left\{\left[\cos(\delta t_1\Omega_0)-1\right]\langle n_j(0)n_j(t_0)n_j(0)\rangle + \langle n_j(t_0)n_j(0)\rangle\right\}\\ &\quad + \left[\sin^2(\delta t_2\Omega_0)+\sin^2(\delta t_1\Omega_0)\right]\langle n_j(t_0)\rangle + \sin^2(\delta t_1\Omega_0)\left[\cos(\delta t_2\Omega_0)-1\right]\langle c_j^\dagger(0)c_j(t_0)c_j^\dagger(t_0)c_j(0)\rangle \qquad (1)\\ A(\delta t_1,\delta t_2) &= 2\sin(\delta t_1\Omega_0)\sin(\delta t_2\Omega_0)\cos(\delta t_2\Omega_0)\Re\left\{e^{-i(\varepsilon_M-\varepsilon_I)t_0/\hbar}\left[\underbrace{\langle c_j^\dagger(t_0)c_j(0)\rangle}_{=:A_1} + (\cos(\delta t_1\Omega_0)-1)\underbrace{\langle n_j(0)c_j^\dagger(t_0)c_j(0)\rangle}_{=:A_2}\right]\right\}\end{aligned}$$

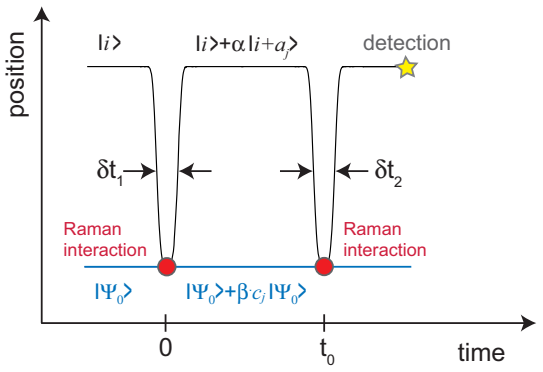

FIG. 3: Schematics of the experimental sequence for the tunnelling mode. The atomic ion $|i\rangle$ is introduced at the lattice site j into the many-body system in state $|\Psi_0\rangle$. The two-photon Raman process (red) couples an atom at this lattice site $|a_j\rangle$ to the ion with a certain amplitude. Subsequently, the ion and the many-body system are separated for the probe time t_0 during which they evolve individually. After recombination, the Raman interaction is applied again and the molecule formation is detected.

We supressed the spin index and on the right hand side additionally the index F.

Using appropriate measurement sequences different correlation functions can be extracted. To obtain the temporal correlation function $\langle c^\dagger_{\sigma,j}(t_0)c_{\sigma,j}(0)\rangle_F$ the described measurement procedure is applied sequentially: first, using $\delta t_1 = \delta t_2 = \delta t$ for both pulses, second using $\delta t_1 = \delta t$ for the first pulse and $\delta t_2 = 2\pi/\Omega_{\sigma,0} - \delta t$ for the second pulse. Subtracting the outcome for the molecule formation of the two measurements gives $\Delta\langle M^\dagger_\sigma M_\sigma\rangle = 2A(\delta t,\delta t)$. For small values of $(\delta t\Omega_{\sigma,0})$ the pre-factor of the first summand A_1 in $A(\delta t,\delta t)$ is quadratic in $(\delta t\Omega_{\sigma,0})$, whereas the prefactor of the second term A_2 is quartic. Since additionally in many systems the decay of the correlation function $\langle n_{\sigma,j}(0)c^\dagger_{\sigma,j}(t_0)c_{\sigma,j}(0)\rangle$ is faster or comparable to the decay of the single particle correlation function the second term can safely be neglected.

The expression $(\varepsilon_I - \varepsilon_M)t_0/\hbar$ represents the phase difference the atomic ion and the molecular ion collect during the time t_0. In principle this quantity could be zeroed by choosing a suitable combination of the optical lattice field and the ion trapping fields. However, this cancellation is not necessary if $\varepsilon_I - \varepsilon_M \gg U, J$ because then the temporal evolution of the correlation function is encoded simply in the envelope of the detection signal.

One direct application of the cold atom tunnelling microscope would be the identification of the quantum many-body phases of the two dimensional Hubbard model. In addition to the normal (Fermi liquid) quantum fluid of fermions, this model can lead to broken symmetry phases such as an anti-ferromagnet, and a strongly correlated (Mott) insulator. An important and yet open question is whether other more exotic phases can exist in this model, such as inhomogeneous distribution of the density (stripes and checkerboards) or even superconducting phases with d-wave symmetry for the pairing. Our local probe directly detects symmetry broken phases such as the anti-ferromagnet in which the spin density is modulated (cf. Fig. 1) and even more inhomogeneous phases with a modulation of the density (stripes and checkerboards [20]).

Additionally, even for phases with homogeneous density and spin density, such as a quantum fluid or a superconductor, the 'tunnelling mode' reveals the nature of the excitations by probing the single particle density of states. This, for example, allows to characterize directly an s-wave or a d-wave superconductor. In Fig. 4 we plot the Fourier transform of the correlation function $\langle c^\dagger_{\sigma,j}(t_0)c_{\sigma,j}(0)\rangle_F$ for both an s-wave superconducting and a d-wave superconducting phase on a two-dimensional lattice. Both are obtained using the phenomenological BCS-approach using the energy dispersion on the lattice $-2J(\cos(k_x a) + \cos(k_y a))$. In the s-wave superconduct-

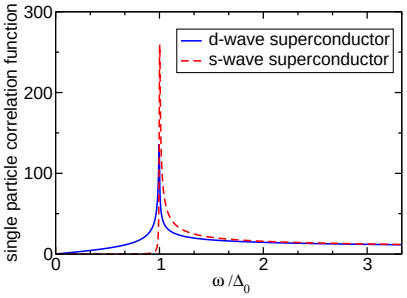

FIG. 4: The Fourier transform of the temporal correlation function in an s-wave and a d-wave superconducting state is shown for a gap value of $\Delta_0 = 0.3J$.

ing phase, the gap $\Delta_s(k) \equiv \Delta_0$, clearly leads to a strong divergence of the correlation signal and a zero response in the gap below Δ_0. For the d-wave superconducting phase with $\Delta_d(k) = \frac{\Delta_0}{2}(\cos(k_x a) - \cos(k_y a))$ [21], one observes a quite different signal having a spectral weight below the gap energy. Thereby the structure of the superconducting order parameter and the size of the gap can be extracted from the proposed measurement.

The independent control over the single particle and the neutral atomic quantum gas lies at the heart of the cold atom tunnelling microscope. To a good approximation the ion experiences only the ion trapping potential, the atom only the optical lattice potential and the weakly bound molecular ion both potentials. This makes the single ion a particularly attractive choice for shuttling the atomic and the molecular ion in and out of the lattice without influencing the neutral atomic quantum many-body state. For example a displacement of 1.2 mm within 50 μs has been achieved without exciting vibrational quanta [22].

The binding energies of the weakly bound states of the atom-ion interaction potential (see Fig. 2) are determined by its asymptotic behavior scaling as $-C_4/r^4$. Here C_4 is proportional to the electric dipole polarizability of the neutral atom and r is the internuclear separation. The binding energy of the most weakly bound molecular state is two orders of magnitude less than for typical neutral atom interactions [23, 24]. Several more deeply bound states with binding energies in the 10-100 MHz range are available for Raman photo-association [25]. The generation of weakly bound molecules using two-photon Raman coupling in optical lattices has already been demonstrated for pairs of neutral atoms [26] and even the coherent coupling of free atomic and bound molecular states has been observed [27] which is the prerequisite for the tunneling mode.

In order to probe the quantum many-body state without perturbations the time scales set by the parameters of the atomic system should be larger than the time intervals of the Raman pulses. To realize a strongly correlated phase in the lattice, the atom-atom scattering length a_{aa} needs to be enhanced by a Feshbach resonance. Assuming $a_{aa} \approx a_{ai} \approx 10^3\, a_0$ results in $U \simeq U_{ai} \simeq 20\,\mathrm{kHz}$ for the fermionic isotope ^{40}K, whereas J is typically one order of magnitude smaller. Therefore the condition for the proposed 'scanning' mode J, U, $U_{ai} \ll 1/\delta t$ can for example be fulfilled using an effective Raman coupling $\Omega_{\sigma,0} = 2\pi \times 10\,\mathrm{kHz}$ applied over a time interval $\delta t = 5\,\mu$s resulting in a molecule formation probability of ≈ 0.1. For the 'tunnelling' mode the Raman coupling needs to be one order of magnitude stronger since the above condition has to be fulfilled for both Raman pulses of duration δt and $2\pi/\Omega_{\sigma,0} - \delta t$, respectively. The shortness of the photo-association pulse has other direct benefits: first, the level shift due to the interaction U_{ai} is not resolved and thus the measurement is independent of the occupation of the lattice well by an atom in the second hyperfine state which is not probed in the spin-resolved mode. Secondly, the short pulse and the subsequent removal of the molecular ion from the quantum many-body system ensures also the stability of the microscope scheme against three-body recombination in a lattice well.

In conclusion, we have proposed a novel experimental setup, the cold atom tunnelling microscope, to observe *locally* the (spin-resolved) density and the single particle Green's function. In contrast to previous work this measurement procedure does not average over spatially different regions of the system with coexisting quantum phases, but can resolve single lattice wells. A modification of the proposed scheme would give also access to *nonlocal* single particle correlation functions. The required modification consists of moving the probe particle during the tunnelling mode scheme to a different lattice well, say m, before the second Raman pulse is applied. The outcome of the molecule formation then will be related to the correlation function $\langle c^\dagger_{\sigma,m}(t_0) c_{\sigma,j}(0)\rangle_F$ of the atomic system. Additionally the proposed setup opens the possibility to create single particle excitations in a controlled way.

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